

James F. Wishart

<http://www.chemistry.bnl.gov/SciandTech/PRC/wishart/wishart.html>

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Positions Held

Senior Chemist

Department of Chemistry, Brookhaven National Laboratory, Upton, New York
September 1987 to present

Assistant Chemist, 1987-1989. Associate Chemist, 1989-1992. Chemist, 1992-2011. Principal Investigator in the Photochemistry and Radiation Chemistry Group. Construction Project Manager and Facility Supervisor of the Laser-Electron Accelerator Facility (LEAF). Research interests include ionic liquids (physical properties of and chemical reactivity within, including charge transport processes and radiation chemistry), long-distance electron transfer, energy and electron transfer in dendrimers, studies of electron transfer and substitution mechanisms using high-pressure techniques, the reactivity of energetic inorganic species, and the development of new accelerators and new detection techniques in pulse radiolysis.

Co-editor, "Photochemistry and Radiation Chemistry: Complementary Methods for the Study of Electron Transfer", *Advances in Chemistry Series*, Vol. 254 (1998). Co-editor, "Recent Trends in Radiation Chemistry", World Scientific, Singapore, (2010). Organizer, Tutorial on Radiation Chemistry Principles and Applications, 209th ACS National Meeting, Inorganic Division, Anaheim, CA, April 2, 1995. Co-organizer, Symposium on Complementarity of Photochemistry and Radiation Chemistry in the Study of Electron Transfer, 209th ACS National Meeting, Inorganic Division, Anaheim, CA, April 2-5, 1995. Co-Organizer, Informational Workshop on Chemistry and Applications of Ionic Liquids, BNL, April 7, 2004. Organizer, International Symposium on Ultrafast Accelerators for Pulse Radiolysis, BNL, June 25-28, 2004. Co-Organizer, Symposium on Physical Chemistry of Ionic Liquids, 232nd ACS National Meeting, Physical Division, San Francisco, CA, Sept., 2006. Guest Co-editor, *J. Phys. Chem. B* special issue on "Physical Chemistry of Ionic Liquids", 111 (18), 2007. Consultant, Deutsche Forschungsgemeinschaft Priority Program in Ionic Liquids, 2006 - 2012. Co-organizer, NYRAILS 2007 Workshop on Ionic Liquids, Rutgers University, Nov. 30, 2007. Co-organizer, Symposium on Ionic Liquids, 40th ACS Middle Atlantic Regional Meeting, Queens, NY, May 18 - 19, 2008, Member, International Advisory Committee, Third International Conference on Ionic Liquids (COIL-3) Cairns, Australia, May 31 - June 3, 2009, Co-Organizer, Symposium on Physical Chemistry of Ionic Liquids, 239th ACS National Meeting, Physical Division, San Francisco, CA, March, 2010, Member, Host Program Committee, Fourth International Conference on Ionic Liquids (COIL-4), Bethesda, MD, June 15-19, 2011.

Postdoctoral Research Fellow

Department of Chemistry, Rutgers, the State University of New Jersey, New Brunswick, NJ
January 1985 to August 1987

In association with Prof. Stephan Isied. Constructed an excimer and dye laser flash photolysis system with cryostat and Macintosh-based control and data analysis system. Investigated long distance electron transfer in cytochrome *c* using covalently-linked ruthenium polypyridine complexes, and the rates of electron transfer across rigid oligopeptide bridges as a function of distance. Conducted enthalpy measurements on the binding of platinum and ruthenium complexes to nucleotides with Prof. Kenneth Breslauer.

Education

Doctor of Philosophy in Inorganic Chemistry

Stanford University, Stanford, California
September 1979 to January 1985

Research advisor: Professor Henry Taube.
National Science Foundation Graduate Fellow, 1980-83.
Dissertation title: *Thermodynamics of Mononuclear and Binuclear Ruthenium Ammine Complexes*.

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Research topics included substitution and redox thermodynamics of ruthenium complexes, the nature of certain mixed-valence binuclear complexes, and quantitative approaches to back-bonding in ruthenium(II) and osmium(II) compounds. Work involved platinum-group synthesis, electrochemistry, batch, flow, titration and solution calorimetry, substitution and electron transfer kinetics, X-ray crystallography, and computerized data acquisition and analysis. Member, University Graduate Housing and Chemistry Department Safety Committees. Supervised two undergraduate research associates.

Bachelor of Science in Chemistry

Massachusetts Institute of Technology, Cambridge, Massachusetts
September 1976 to June 1979

Supplemented the standard curriculum with graduate courses in molecular spectroscopy, advanced inorganic chemistry, and organometallic chemistry. Humanities concentration was Art. Served as vice president and treasurer of my dormitory and on the New Undergraduate Housing Committee. Undergraduate research was done during the summers of 1978 and 1979 with Prof. Richard Lintvedt at Wayne State University in my hometown of Detroit.

Teaching and Mentoring Experience

BNL: Recipient, U. S. DOE Office of Science Outstanding Mentor Award, Feb. 2006. Keynote Lecturer, 54th ACS New York Section Undergraduate Research Symposium, St. John's University, Queens, NY, April 29, 2006. Mentored DOE Office of Educational Programs Faculty and Student Teams (FaST) each summer 2003-2007; was the first to host FaST team at BNL, 2003. Since 2003, mentored a total of 23 undergraduates, one graduate and three junior faculty in programs sponsored by DOE OEP (FaST, SULI, CCI), BNL Diversity Office, NIH, and SUNY Stony Brook (Battelle-WISE Fellowship), for a total of 44 person-summers. **Instructor:** 2009 OEP Mini-Semester course (for 23 college students) on ionic liquids, radiation chemistry, chemical kinetics and the LEAF accelerator facility (Jan. 12-16, 2009). Gave lectures, supervised laboratory activities and guided students through sample preparation, pulse radiolysis measurements, data analysis and report generation on a real research problem involving reaction kinetics in ionic liquids.

Stanford University: Teaching Assistant, first quarter Inorganic Chemistry, for Keith Hodgson, Winter 1984 (Gave a ninety-minute lecture on substitution and electron transfer mechanisms). Lecturer and TA, second quarter Inorganic Chemistry, with Henry Taube and Keith Woo, Spring 1982 (Gave nine lectures (1/3 of the course) on ligand field theory, molecular orbital theory, transition metal spectroscopy, and magnetism. Shared administrative responsibility for the course). TA, first quarter Inorganic Chemistry, for Keith Hodgson, Winter 1982. TA, second quarter Inorganic Chemistry, for Henry Taube, Spring 1981. Head TA, second quarter Organic Chemistry, for K. Barry Sharpless, Spring 1980 (Prepared demonstrations, collaborated in test preparation and final grading). TA, Analytical Laboratory, for Keith Hodgson, Winter 1980. TA, General Chemistry, for Hans C. Andersen, Fall 1979.

Other Experience

Research Assistant, Wayne State University, Detroit, MI, June to September, 1978 and 1979 with Prof. Richard Lintvedt. Studied dicopperbistriketonates and related molecules. Performed original organic and inorganic synthesis and non-aqueous electrochemistry. Designed a new triketone that led to a novel series of complexes.

Additional Information

Member, American Chemical Society (Inorganic and Physical Divisions), American Association for the Advancement of Science, and Miller Trust for Radiation Chemistry.

References: Available upon request.

List of Publications

- Synthesis, Structure, and Magnetism of a New Type of π -Molecular Complex Containing Binuclear Copper(II) Complexes and Benzene: Bis[2,2-dimethyl-7-(phenylimino)-3,5,7-octanetrionato]dicopper(II)-Benzene and Bis[2,2-dimethyl-7-((4-nitrophenyl)imino)-3,5,7-octanetrionato]dicopper(II)-Bis(benzene)*
J. F. Wishart, C. Ceccarelli, R. L. Lintvedt, J. M. Berg, D. P. Foley, T. Frey, J. E. Hahn, K. O. Hodgson and R. Weis
Inorg. Chem. **22**, 1667-1671 (1983)
- Enthalpies of Reaction of Pentaammineruthenium(II) Complexes*
J. F. Wishart, H. Taube, K. J. Breslauer and S. S. Isied *Inorg. Chem.* **23**, 2997-3001 (1984)
- Backbonding Effects of Osmium(III): The Crystal Structure of μ -Pyrazinedecaamminediosmium(II) Chloride Dihydrate*
A. Bino, P. A. Lay, H. Taube and J. F. Wishart *Inorg. Chem.* **24**, 3969-3971 (1985)
- The Enthalpy of Formation of Nitrosylpentaammineruthenium(II) from NO^{+} (aq) and Aquopentaammineruthenium(II)*
J. F. Wishart, H. Taube, K. J. Breslauer and S. S. Isied *Inorg. Chem.* **25**, 1479-1481 (1986)
- A Very Short Ruthenium(II) - Nitrogen Heterocycle Bond: The Crystal Structures of Pentaammine(N-methylpyrazinium)ruthenium(II) Iodide and Pentaammine(N-methylpyrazinium)ruthenium(III) p-Toluenesulfonate Pentahydrate*
J. F. Wishart, A. Bino and H. Taube *Inorg. Chem.* **25**, 3318-3321 (1986)
- The Distance Dependence of Intramolecular Electron-Transfer Rates: Importance of the Nuclear Factor*
S. S. Isied, A. Vassilian, J. F. Wishart, C. Creutz, H. A. Schwarz and N. Sutin
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- A Dissociative Pathway for Equilibration of a Hydrido $CoL(H)^{2+}$ Complex with CO_2 and CO : Ligand Binding Constants in the Macroyclic [14]Dienecobalt(I) System*
C. Creutz, H. A. Schwarz, J. F. Wishart, E. Fujita and N. Sutin *J. Am. Chem. Soc.* **111**, 1153-1154 (1989)
- Arene-to-Alkyne Linkage Isomerizations of Diphenylacetylene on Pentaammineosmium*
W. D. Harman, J. F. Wishart and H. Taube *Inorg. Chem.* **28**, 2411-2413 (1989)
- Report of the Workshop on the Proposed Pulse Radiolysis Facility at Brookhaven National Laboratory*
C. Creutz, H. A. Schwarz and J. F. Wishart BNL Report, BNL-52229, (1989)
- Electron Transfer Across Polypeptides. 6. Long Range Electron Transfer in Osmium-Ruthenium Binuclear Complexes Bridged with Oligoproline Peptides*
A. Vassilian, J. F. Wishart, B. van Hemelryck, H. Schwarz and S. S. Isied
J. Am. Chem. Soc. **112**, 7278-7286 (1990)
- Thermodynamics and Kinetics of Carbon Dioxide Binding to Two Stereoisomers of a Cobalt(I) Macrocycle in Aqueous Solution*
C. Creutz, H. A. Schwarz, J. F. Wishart, E. Fujita and N. Sutin *J. Am. Chem. Soc.* **113**, 3361-3371 (1991)
- High Pressure Pulse Radiolysis. Modification of an Optical Cell for 2-MeV Electron Pulse Radiolysis at Pressures up to 200 MPa*
J. F. Wishart and R. van Eldik *Rev. Sci. Instrum.* **63**, 3224-3225 (1992)
- High-Pressure Pulse Radiolysis Study of Intramolecular and Intermolecular Reduction of Cytochrome c by Ruthenium(II) Ammine Complexes*
J. F. Wishart, R. van Eldik, J. Sun, C. Su and S. S. Isied *Inorg. Chem.* **31**, 3986-3989 (1992)

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Molecular and Electronic Structure of the Electron-Transfer Probe Analogue

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J. F. Wishart, X. Zhang, S. S. Isied, J. A. Potenza and H. J. Schugar *Inorg. Chem.* **31**, 3179-3181 (1992)

Peptide-Mediated Intramolecular Electron Transfer: Long-Range Distance Dependence

S. S. Isied, M. Y. Ogawa and J. F. Wishart *Chem. Rev.* **92**, 381-394 (1992)

Distance Dependence of Intramolecular Electron Transfer Scross Oligoprolines in

[(bpy)₂Ru^{II}L[•]-(Pro)_n-Co^{III}(NH₃)₅]³⁺, n = 1-6: Effect of the Helical Polyproline II Structure

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Long Range Electron Transfer in Helical Polyproline II Oligopeptides

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C. Fenwick, S. Marmor, K. Govindaraju, A. M. English, J. F. Wishart and J. Sun

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Electron Transfer from the Heme of Cytochrome c to Two Equidistant Redox-Modified Sites, Histidine 33 and Methionine 65: The Importance of Electronic Effects and Peptide Networks

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Proc. Nat. Acad. Sci. **93**, 9521-9526 (1996)

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J. E. Roberts, D.-N. Hu, and J. F. Wishart *J. Photochem. Photobiol. B: Biology* **42**, 125-132 (1998)

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J. Zhou, M. A. Case, J. F. Wishart and G. L. McLendon *J. Phys. Chem. B* **102**, 9975-9980 (1998)

Site-Dependent Stereoselective Binding of Ruthenium Aquobipyridine Complexes to Histidine Side Chains in Horse Heart Cytochrome c

J. Luo, J. F. Wishart and S. S. Isied *J. Am. Chem. Soc.* **120**, 12970-12971 (1998)

High Enantioselectivity in the Electron Transfer Reaction between a Ru(II) Complex of Menbpy Anion Radical, [Ru(menbpy)₃]⁺ [menbpy=4,4'-di{(1R,2S,5R)-(-)-menthoxy carbonyl}-2,2'-bipyridine] and [Co(acac)₃]: A Pulse Radiolysis Study

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The Brookhaven Laser-Electron Accelerator Facility (LEAF)

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De Novo Design of Protein Function: Predictable Structure-Function Relationships in Synthetic Redox Proteins M. W. Mutz, M. A. Case, J. F. Wishart, M. R. Ghadiri and G. L. McLendon
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T. Hamada, B. S. Brunschwig, K. Eifuku, E. Fujita, M. Körner, S. Sakaki, R. van Eldik and J. F. Wishart
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A. Y. Kornilova, J. F. Wishart, W. Xiao, R. C. Lasey, A. Fedorova, Y.-K. Shin, and M. Y. Ogawa
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